Model of coarsening and vortex formation in vibrated granular rods

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Neicu *et al.* observed experimentally spontaneous formation of the long-range orientational order and large-scale vortices in a system of vibrated macroscopic rods. We propose a phenomenological theory of this phenomenon based on a coupled system of equations for local rods density and tilt. The density evolution is described by the modified Cahn-Hilliard equation, while the tilt is described by the Ginzburg-Landau type equation. Our analysis shows that, in accordance with the Cahn-Hilliard dynamics, islands of the ordered phase appear spontaneously and grow due to coarsening. The generic vortex solutions of the Ginzburg-Landau equation for the tilt correspond to the vortical motion of the rods around the cores which are located near the centers of the islands.

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Vibrated granular materials exhibit many interesting phenomena, including formation of cellular and localized patterns, phase separation, etc. [1–6]. Neicu *et al.* [7] studied the dynamics of a layer of long cylindrical grains (rods) subjected to vertical vibration, and discovered a surprising phenomenon of spontaneous formation of ''islands'' of vertically aligned rods which coexist with the ''sea'' of almost horizontal rods. Subsequently, small islands merge and form large islands which typically exhibit collective vortical motion of rods. Near the core this motion has a form of a solid body rotation, while farther away the angular velocity decays. While the bistability and first-order phase transitions leading to phase separation and coarsening are typical in granular dynamics and usually caused by the inelasticity of grains [2–6,8], the emergence of the vortical motion within the ordered phase is unexpected. Experiment [7] shows that rods within a vortex are tilted in the azimuthal direction, and slowly drift in the direction of the tilt. Neicu *et al.* [7] suggested that the drift occurs due to the confinement of the rod vibration by its tilted neighbors.

In this article we introduce a continuous phenomenological model of the transition to the ordered vortical state based on the modified Cahn-Hilliard equation governing the dynamics of local rods density and the Ginzburg-Landau type equation for the tilt. Our model reproduces qualitatively the observed phase separation, coarsening and vortex formation. We derive the solutions for the stationary vortices and discuss their stability.

Model. The motion of rods is described by the momentum conservation equation in the form

$$\rho\left(\frac{D\mathbf{v}}{Dt}+\zeta\mathbf{v}\right)=-\nabla p+\alpha\mathbf{n}f_0(n)\rho. \qquad (1)$$

Here $\mathbf{v}=(v_x,v_y)$ is the horizontal velocity of rods, ρ is the density, p is the hydrodynamic pressure, the tilt vector $\mathbf{n}=(n_x,n_y)$ is the projection of the rod director on the (x,y) plane, and $n=|\mathbf{n}|$. The term $\alpha\mathbf{n}f_0(n)\rho$ accounts for the average driving force from the vibrating bottom on the tilted rod. According to experiments [7], the driving force is proportional to the tilt of rods for small tilt values, but saturates and eventually decays to zero at n. Coefficient α is proportional to the velocity magnitude of the plate oscillations, and so for a fixed acceleration magnitude is inversely proportional to the vibration frequency. For definiteness we set $f_0=\alpha_1-n^2$, with $\alpha_1=\text{const}$ (the last term in f_0 models decay of driving force for large tilts). The term $\zeta\mathbf{v}$ describes the momentum dissipation due to bottom friction. Equation (1) must be augmented by the mass conservation equation

$$\partial_t\rho+\text{div}(\mathbf{v}\rho)=0. \qquad (2)$$

In the following we assume that friction is strong, and neglect the inertia term $D\mathbf{v}/Dt$ with respect to the friction term $\zeta\mathbf{v}$. Thus, we can express the velocity in the form

$$\mathbf{v}=-[\nabla p-\alpha\mathbf{n}f_0(n)\rho]/\zeta\rho. \qquad (3)$$

Now, substituting the velocity (3) into the mass conservation law, Eq. (2), we obtain

$$\partial_t\rho=\zeta^{-1}\,\text{div}[\nabla p-\alpha\mathbf{n}f_0(n)\rho]. \qquad (4)$$

To describe phenomenologically the observed phase separation and coarsening we employ the Cahn-Hilliard approach (see Ref. [10] for review). We assume that the pressure p can be obtained from the variation of a ''free energy'' functional of the ρ field $p=\delta F/\delta\rho$. We adopt the standard form of the free energy taking into account the local dynamics and diffusive-type spatial coupling

$$F=\int\int dxdy\left(\frac{l^2}{2}(\nabla\rho)^2+f(\rho)\right), \qquad (5)$$

where l is the length scale related to the rod size. To be able to exhibit phase separation, function f should have two minima separated by a maximum. We choose a generic cubic polynomial form of $df/d\rho$. Without loss of generality we can write $df/d\rho=(\rho-\rho_0)[\delta_0-\delta_1(\rho-\rho_0)+(\rho-\rho_0)^2]$.

Since $df/d\rho$ is defined up to an additive constant, we can fix the root ρ_0 to be a minimal density for the onset of nematic order. The existence of such a density for the system of rigid rods for equilibrium systems was argued by Onsager [11]. The constants δ_0 and δ_1 are some functions of the driving acceleration. Experimentally, the dense phase nucleates for large enough vertical acceleration. In our description, a minimum in $df/d\rho$ corresponding to the existence of dense phase appears for large δ_1. We will associate δ_1 with acceleration and keep δ_0 fixed. Substituting p with Eq. (5) into Eq. (4), after rescaling we obtain the modified Cahn-Hilliard equation (we replaced ρ by $\rho-\rho_0$ and used the same notations for the rescaled variables $r\to r/l$, $t\to t/\zeta l^2$)

$$\partial_t\rho=-\nabla^2[\nabla^2\rho-\rho(\delta_0-\delta_1\rho+\rho^2)] - \alpha\,\mathrm{div}[\mathbf{n}f_0(n)(\rho+\rho_0)], \tag{6}$$

To close the description we need to add an equation for the evolution of tilt $\mathbf{n}$. For ρ smaller than the maximum packing density the vertical orientation of rods corresponding to $\mathbf{n}=\mathbf{0}$ is unstable, as rods spontaneously tilt. We assume that the growth rate of the instability depends on the rods packing density, so we can write for the local dynamics $\partial_t\mathbf{n}=f_1(\rho)\mathbf{n}-|\mathbf{n}|^2\mathbf{n}$ with $f_1(\rho)=a_0-a_1\rho$, $a_{0,1}>0$ some constants. The last term in f_1 describes the saturation of the instability at smaller values of the equilibrium tilt for larger ρ. In addition, rods interact with each other, which leads to the spatial derivative operator $\hat{D}[\mathbf{n}]$. Since the tilt field is not divergence-free, from the general symmetry considerations, in the lowest (second) order, the "diffusion" operator acting on $\mathbf{n}$, takes the form $\hat{D}[\mathbf{n}]=f_2(\rho)(\xi_1\nabla^2\mathbf{n}+\xi_2\nabla\,\mathrm{div}\,\mathbf{n})$. The coefficients $\xi_{1,2}$ (normalized by ζ) in this expression are analogous to the first and second viscosity in ordinary fluids (see Ref. [9]). Function $f_2(\rho)$ describes the decrease of the spatial coupling strength as the rods density decreases. In the gas phase ($\rho<0$) the spatial coupling between the rods is small and their tilt becomes large and uncorrelated. Accordingly, we set $f_2=\rho$, if $\rho>0$ and $f_2=0$ otherwise. Finally, we include the simplest term describing coupling between the tilt and the density gradient $\beta\boldsymbol{\nabla}\rho$. Combining all these terms we arrive at

$$\partial_t\mathbf{n}=f_1(\rho)\mathbf{n}-|\mathbf{n}|^2\mathbf{n}+f_2(\rho)(\xi_1\nabla^2\mathbf{n}+\xi_2\boldsymbol{\nabla}\,\mathrm{div}\,\mathbf{n})+\beta\boldsymbol{\nabla}\rho. \tag{7}$$

It is convenient to introduce new complex variable $\psi=n_x+in_y$. Then, Eq. (7) assumes the form of the generalized Ginzburg-Landau equation ($\bar{\xi}=\xi_1+\xi_2/2$)

$$\partial_t\psi=(f_1(\rho)-|\psi|^2)\psi+\beta(\partial_x+i\partial_y)\rho + f_2(\rho)\left(\bar{\xi}\nabla^2\psi+\frac{\xi_2}{2}(\partial_x+i\partial_y)^2\psi^*\right). \tag{8}$$

For large δ_1 Eq. (6) exhibits *phase separation* in a certain range of the filling fraction defined as $\Phi=S^{-1}\int\int\rho\,dx\,dy$, where S is the cavity area. Stationary uniform solutions to Eq. (6) obey

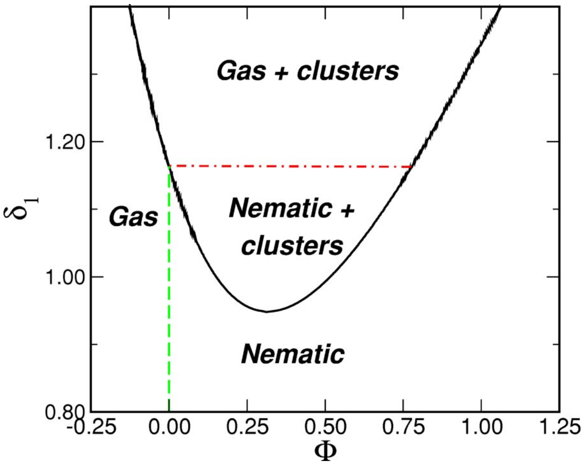

FIG. 1. Phase diagram for $\delta_0=0.3$. Above the solid curve high and low-density phases coexist, below there are only single-phase solutions, "nematic" for $\Phi>0$ and gas otherwise.

$$\rho(\delta_0-\delta_1\rho+\rho^2)=B, \tag{9}$$

where $B=$const is determined below. In the phase separation regime Eq. (9) has three real roots $\rho_1<\rho_2<\rho_3$ (ρ_2 corresponds to the unstable solution and $\rho_{1,3}$ to the stable ones). The phase separation leads the high-density phase domains $\rho=\rho_3$ of the area S_h and the low-density one $\rho=\rho_1$ of the area $S_l=S-S_h$. From the mass conservation one obtains

$$S_h\rho_3+(S-S_h)\rho_1=S\Phi. \tag{10}$$

Here we neglected the interfacial contributions assuming that S_l, $S_h\gg 1$. In addition, Eq. (10) must be augmented by the condition that the free energy densities of the both phases are equal, which is expressed by the relation (so-called area rule, see e.g., Ref. [12])

$$\int_{\rho_1}^{\rho_3}[\rho(\delta_0-\delta_1\rho+\rho^2)-B)]d\rho=0. \tag{11}$$

Equations (9) and (11) fix the value of B and correspondingly the roots $\rho_{1,3}$. From Eq. (10) it follows that multiphase stable solutions are possible if $\rho_1<\Phi<\rho_3$. This condition defines the transition line shown in Fig. 1. Below this line only single-phase stationary solutions with $\rho=\Phi$ exist. If $\Phi>0$, according to Eq. (8), these solutions have nonzero tilt and fixed phase $\psi=\psi_0\exp[i\phi_0]$, ψ_0, $\phi_0=$const (nematic ordering of the rods), otherwise a gaseous state with no orientational order is formed. Above the transition one expects spontaneous formation of dense clusters with density ρ_3 coexisting with low-density (ρ_1) nematic phase (if $\rho_1>0$) or gas (if $\rho_1<0$).

In addition to the uniform solutions, Eq. (8) admits solutions with nonzero topological charge: defects or vortices. Let us consider radially symmetric *vortex* solutions to Eq. (8). In this case ρ is a function of the polar radius r, and ψ can be expressed as $\psi=\exp(\pm i\theta)w(r)$, where w is a complex function, and θ is the polar angle (for definiteness we take sign $+$). Using $\partial_x+i\partial_y=\exp(i\theta)(\partial_r+i/r\partial_\theta)$, we obtain, from Eq. (8),

$$\partial_t w = f_2\left(\overline{\xi}\nabla_r^2 w + \frac{\xi_2}{2}\nabla_r^2 w^*\right) + f_1 w - |w|^2 w + \beta\rho_r, \tag{12}$$

where $\nabla_r^2 = \partial_r^2 + r^{-1}\partial_r - r^{-2}$ is the radial Laplacian operator. For $\xi_2, \beta = 0$, Eq. (12) possesses a stationary solution in the form $w = W(r)\exp(i\phi_0)$ with the real positive magnitude W and an arbitrary constant phase ϕ_0. The terms $\propto \xi_2, \beta$ still permit the constant phase solutions, but they destroy the continuous phase degeneracy. Indeed, Eq. (12) for $\beta = 0$ yields

$$f_2\left(\overline{\xi} + \frac{\xi_2}{2}\cos 2\phi_0\right)\nabla_r^2 W + f_1 W - W^3 = 0 \tag{13}$$

and $\sin 2\phi_0 = 0$. Solutions exist only for $\phi_0 = 0, \pi$, or $\pm\pi/2$. Function W describes the standard (and well-documented) vortex solution to the Ginzburg-Landau equation with the property $W \to f_1^{1/2}$ for $r \to \infty$ and $W \sim r$ for $r \ll 1$ (for its rational approximation see e.g., Ref. [13]). Solutions with $\phi_0 = 0, \pi$ describe sinks (sources) with zero circulations, whereas the solutions with $\phi_0 = \pm\pi/2$ are vortices with nonzero circulations. The sign of ϕ_0 determines the direction of rotation. Near the vortex core $W \sim r$, which corresponds to the solid body rotation, as velocity $v_\theta \sim W$. Far away from the core the vortex exhibits differential rotation.

For $\beta\partial_r\rho \neq 0$, Eq. (12) has constant phase solutions only with $\phi_0 = 0, \pi$, i.e., with *zero circulation*. However, it does not guarantee the selection of this solution in the bulk of large islands where the density gradient is small. It is easy to show that solutions with $\phi_0 = 0$ are energetically unfavorable with respect to rotating solutions with $\phi_0 = \pm\pi/2$ if $\beta\partial_r\rho$ is small. Equation (12) for $\beta\partial_r\rho = 0$ can be written in the form $\partial_t w = -\delta U/\delta w^*$ with the free energy

$$U = \int d\mathbf{r}\left[f_2\overline{\xi}(|\partial_r w|^2 + r^{-2}|w|^2) + \frac{f_2\xi_2}{4}\{[(\partial_r + r^{-1})w^*]^2 + \text{c.c.}\} - f_1|w|^2 + |w|^4\right]. \tag{14}$$

Substituting vortex solution $w = W(r)\exp(i\phi_0)$ in Eq. (14), one obtains after integration (since the calculation of the vortex energy is rather straightforward, we refer interested readers to Ref. [13], p. 11).

$$U = f_1 f_2(\overline{\xi} + \xi_2/2\cos 2\phi_0)\ln R/r_0 + \text{const}, \tag{15}$$

where $r_0 \sim O(1)$ has the meaning of core radius, and R is the outer cutoff radius of integration. As one sees from Eq. (15), for physically realizable case $\xi_2 > 0$ the vortices with $\phi_0 = \pm\pi/2$ have lower energy, and therefore are more energetically favorable, and are selected in dynamics. In a general case, the vortex solution would have a radius-dependent phase ϕ_0. Near the center where the density is almost constant, the phase would be close to $\pm\pi/2$, and near the island border where the density decreases rapidly, the phase should approach 0 or π. This scenario suggests that the azimuthal velocity should grow with radius near the core, and decrease near edge of the vortex, which is confirmed by our numerical simulations (see below) and agrees with experiments. In addition, one can show that for $\beta > 0$ the term $\beta\nabla\rho$ considered as a small perturbation, leads to the drift of the vortex core towards the gradient of density, and therefore it stabilizes the vortex core near the center of the island. Note that topological defects exist also in the nematic phase. However, in the nematic phase tilt is large and, correspondingly, the hydrodynamic velocity is small, so the nematic defects do not form hydrodynamic vortices.

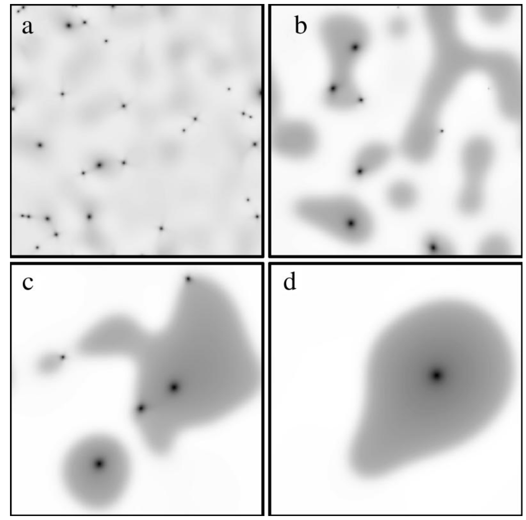

FIG. 2. Evolution of $|\psi|$, vortices are shown as black dots, white area corresponds to larger $|\psi|$ (and ρ), dark vice versa. Parameters, $\overline{\xi} = 1$, $\xi_2 = 1$, $\beta = 0.04$, $f_0 = 1.5 - |\psi|^2$, $f_1 = 1.4 - 0.7\rho$, $\delta_1 = 1.3$, $\delta_0 = 0.3$, $\rho_0 = 0.25$, $\alpha = 0.03$. Images are shown for $t = 80$ (a), 400 (b), 1600 (c), and $t = 3200$ (d).

Numerical simulations of the Cahn-Hilliard equation (6) were performed using an FFT split-step method, and the Ginzburg-Landau equation (8) was solved using explicit method. The domain of integration was 100×100 dimensionless units with periodic boundary conditions, number of FFT harmonics was 256×256. As initial conditions we used $\rho \approx \rho_2$ with small amplitude noise and random initial conditions for ψ. Selected results are presented in Figs. 2–4.

At the initial stage of the evolution, many vortices and small dense clusters (islands) are created throughout the domain of integration [Fig. 2(a)]. Islands are seen as darker areas on the figure, because an increase in density ρ results in the decrease of $|\psi|$. Some islands trap vortices and are practically immobile, others do not contain vortices and drift in the direction defined by the average orientation of the tilt $\mathbf{n}$. With time, small islands disappear and bigger islands grow [Fig. 2(b),(c)]. It is interesting to note that due to the tilt-driven drift coarsening occurs much faster than in the ordinary Cahn-Hilliard dynamics. Finally, one big island with the vortex in the center is formed [Fig. 2(d)]. Density ρ, tilt amplitude $|\psi|$, the phase arg ψ, and the velocity field of a quasistationary vortex are shown in Fig. 3. Even far from the island there are some "dormant vortices" in the low-density phase (gas). These defects are seen as the end points of the phase singularity lines (lines between dark and white) in Fig.

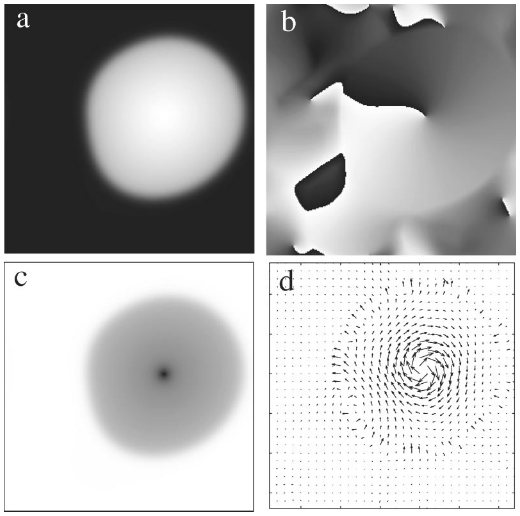

FIG. 3. Density ρ (a), phase arg ψ (b), tilt amplitude $|\psi|$ (c), and velocity field for $t=4960$, other parameters as in Fig. 2. Black corresponds to $\rho=0=\arg\psi=|\psi|=0$, white to $\rho=1.4$, $\arg\psi=2\pi$, $|\psi|=1.2$.

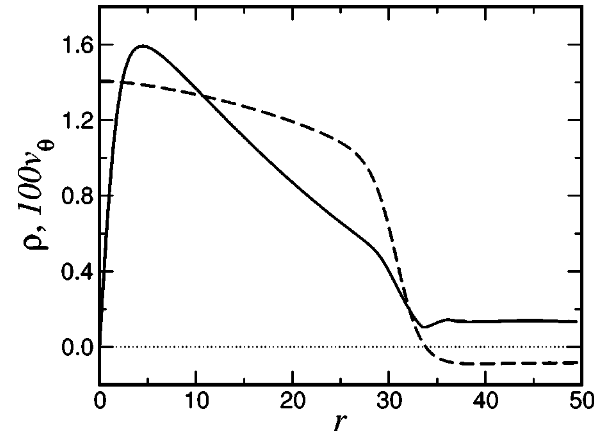

FIG. 4. Azimuthal velocity v_θ (solid line) and density ρ (dashed line) vs r for the parameter of Fig. 2.

3(b). They do not annihilate because in the low-density phase the diffusion terms in Eq. (8) are absent. They are not seen in Fig. 3(c), because their core size is small in the gas phase. Figure 3(d) shows the corresponding velocity field calculated using Eq. (3). Rods perform circular motion around the vortex center. The azimuthal velocity v_θ vs r is shown in Fig. 4. The velocity is maximal somewhere between the core and the island edge. It qualitatively resembles the experimental one [7]. Outside the island the tilt becomes large and the velocity becomes small. The magnitude of azimuthal velocity is proportional to α, and, therefore, inversely proportional to the vibration frequency, in agreement with experiment.

In conclusion, we developed a phenomenological model of the formation of the vortical ordered state in the system of vertically vibrated rods. The model reproduces qualitative features of the vortex formation process observed in the recent experiment [7]. Note that in our theory the tilt of rods in a single-phase regime (at low δ_1) is determined by the density, so high filling fraction automatically implies almost vertical rod packing even without driving. In the experiment, the initial high filling fraction configuration corresponded to a thick layer of randomly packed almost horizontal rods. This makes it difficult to compare the phase diagram, Fig. 1, to the experimental one for high filling fraction, although qualitatively it correctly described the transition to phase separation regime with the increasing "vibration magnitude" δ_1. We thank Toni Neicu, Daniel Blair, and Arshad Kudrolli for stimulating discussions.

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